STABILITY AND ABSENCE OF BINDING FOR MULTI-POLARON SYSTEMS

RUPERT L. FRANK, ELLIOTT H. LIEB, ROBERT SEIRINGER,
AND LAWRENCE E. THOMAS

ABSTRACT. We resolve several longstanding problems concerning the stability and the absence of multi-particle binding for $N \geq 2$ polarons. Fröhlich's 1937 polaron model describes non-relativistic particles interacting with a scalar quantized field with coupling $\sqrt{\alpha}$, and with each other by Coulomb repulsion of strength U. We prove the following: (i) While there is a known thermodynamic instability for $U < 2\alpha$, stability of matter *does* hold for $U > 2\alpha$, that is, the ground state energy per particle has a finite limit as $N \to \infty$. (ii) There is no binding of any kind if U exceeds a critical value that depends on α but not on N. The same results are shown to hold for the Pekar-Tomasevich model.

1. INTRODUCTION AND MAIN RESULTS

Fröhlich's large polaron [9] is a model for the motion of an electron in a polar crystal and it is also relevant as a simple model of non-relativistic quantum field theory. Consequently there is a huge literature, both experimental and theoretical, devoted to its study. See, e.g., [12, 32, 31, 27, 1] and references therein. Our concern here is with the binding or non-binding of several polarons: whether the ordinary Coulomb repulsion among the electrons can, if strong enough, prevent the binding that would otherwise be created by the electric field of the polar crystal. We are also interested in the *stability of matter*, i.e., whether the energy of N polarons is bounded below by a constant times N even when there is binding.

In this model the single polaron, which is one non-relativistic electron interacting with a phonon field, has the Hamiltonian

$$H^{(1)} = p^2 - \sqrt{\alpha}\phi(x) + H_f \,. \tag{1.1}$$

This Hamiltonian acts in the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathcal{F}$, where $\mathcal{F}$ is the bosonic Fock space for the longitudinal optical modes of the crystal, with scalar creation and annihilation operators $a^\dagger(k)$ and $a(k)$ satisfying $[a(k), a^\dagger(k')] = \delta(k - k')$. The electron momentum is $p = -i\nabla$, the phonon field energy is

$$H_f = \int_{\mathbb{R}^3} dk \, a^\dagger(k)a(k) \,, \tag{1.2}$$

and the interaction of the crystal modes with the electron is

$$\phi(x) = \frac{1}{\sqrt{2}\pi} \int_{\mathbb{R}^3} \frac{dk}{|k|} \left(e^{ikx}a(k) + e^{-ikx}a^\dagger(k) \right) \,, \tag{1.3}$$

with coupling constant $\alpha > 0$. (In another frequently used convention α is replaced by $\alpha/\sqrt{2}$.) The ground state energy $E^{(1)}(\alpha)$ is the infimum of the spectrum of $H^{(1)}$. Because of translation invariance, $E^{(1)}(\alpha)$ cannot be expected to be an eigenvalue, and indeed it is not; this was proved in [11] using methods developed in [10].

A noteworthy feature of the phonon field energy H_f is its flat dispersion relation, i.e., there is no non-constant function $\omega(k)$ in the integrand of (1.2). The energy of infrared phonons does not go to zero as $|k| \to 0$, while the ultraviolet energy is finite when $|k| \to \infty$. If we tried to minimize the energy in a naïve way by completing the square, we would end up with a Coulomb-like $\int dk\, |k|^{-2}$ self-energy of the polaron. The non-integrability for large k would lead to a divergent self-energy, but this divergence is actually mitigated by the electron kinetic energy p^2 and the uncertainty principle. While the single polaron has finite energy, another problem remains for the many-polaron system; the energy is finite, but stability of matter will not hold unless a sufficiently strong Coulomb repulsion among the electrons is included in the Hamiltonian.

The Hamiltonian for N electrons is

$$H_U^{(N)} = \sum_{i=1}^{N} \left(p_i^2 - \sqrt{\alpha}\phi(x_i) \right) + H_f + U\, V_C(X) \tag{1.4}$$

with $X = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$ and

$$V_C(X) = \sum_{i<j} \frac{1}{|x_i - x_j|}. \tag{1.5}$$

We impose no symmetry restrictions on the electrons, which means that our lower bounds apply equally to bosons or fermions or particles with no symmetry restrictions (boltzons). The Hilbert space is then $L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}$. Particle spin is irrelevant for our results and is ignored. Physically, the parameter U is the square of the electron charge, and it satisfies $U > 2\alpha$ [9]. Nevertheless, we will consider all values $U \geq 0$.

The ground state energy of $H_U^{(N)}$ is denoted by $E_U^{(N)}(\alpha)$, and the *binding energy* is defined to be $\Delta E_U^{(N)}(\alpha) = N E^{(1)}(\alpha) - E_U^{(N)}(\alpha)$. We will prove three theorems about these quantities. They were previously summarized in an announcement [8]. Our main goal is to find conditions on U and α such that no binding occurs, i.e., $\Delta E_U^{(N)}(\alpha) = 0$. Of particular physical interest is the case $N = 2$ (*bipolaron*).

Theorem 1 (Absence of binding for N polarons). *For given $\alpha > 0$ there is a finite $U_c(\alpha) > 2\alpha$ such that*

$$\Delta E_U^{(N)}(\alpha) = 0 \quad \text{for all } N \geq 2 \tag{1.6}$$

whenever $U \geq U_c(\alpha)$.

Our proof is constructive and gives an explicit upper bound on $U_c(\alpha)$; see the discussion at the end of Section 4. This bound on $U_c(\alpha)$ is linear in α for large α, which is the correct behavior. Presumably, the true $U_c(\alpha)$ behaves linearly even for small α, but this remains an *open problem*.

For the bipolaron, $N = 2$, our proof is simpler and yields the sharper result that the critical $U_c(\alpha)$ indeed obeys a linear law:

Theorem 2 (Absence of binding for bipolarons). *Let $N = 2$. For some constant $C < 26.6$,*

$$\Delta E_U^{(2)}(\alpha) = 0 \tag{1.7}$$

whenever $U \geq 2C\alpha$.

The optimal constant C in Theorem 2 is presumably much closer to 1 than the bound we derive. It is not equal to 1, however. In the strong coupling limit $\alpha \to \infty$, binding occurs if $U \leq 2.3\,\alpha$ [33, 31]. For small α, on the other hand, variational calculations [33, 2] suggest that bipolaron binding does not occur at all for any $U \geq 2\alpha$. The proof of this remains an *open problem*.

On the other hand, if binding does occur, we would like to know how the binding energy depends on N; in particular, is there *stability of matter*, in the sense that $\Delta E_U^{(N)}(\alpha) \leq C(U, \alpha)N$ for all N?

This linear bound, if it exists, implies the existence of the *thermodynamic limit*

$$\lim_{N \to \infty} N^{-1} E_U^{(N)}(\alpha)\,.$$

The proof is a simple consequence of the sub-additivity of the energy, i.e.,

$$E_U^{(N+M)}(\alpha) \leq E_U^{(N)}(\alpha) + E_U^{(M)}(\alpha)\,, \tag{1.8}$$

which follows from the fact that one can construct variational functions in which N electrons are localized on the earth and M behind the moon [13] [20, Sec. 14.2].

The proof of the linear lower bound is far from obvious; indeed, it is not always true! Griesemer and Møller [13] recently proved that when $U < 2\alpha$, there are positive constants (depending on U and α) such that $-c_1 N^{7/3} \geq E_U^{(N)}(\alpha) \geq -c_2 N^{7/3}$. This result holds for particles, like electrons, that satisfy Fermi statistics. If the electrons were bosons, the result would be even worse, $-N^3$, as a similar analysis shows. This is the same behavior as that of gravitating particles in stars [20, Ch. 13]. In the opposite regime, $U > 2\alpha$, [13] shows that $E_U^{(N)}(\alpha) \geq -C(U, \alpha)N^2$, independently of statistics, where $C(U, \alpha) \to \infty$ as $U \searrow 2\alpha$. (In their convention the dividing line is $U = \sqrt{2}\alpha$.)

Judging from the physics of the model, it is reasonable to suppose that there is a linear law as soon as $U > 2\alpha$. This we are able to prove.

Theorem 3 (Stability for $U > 2\alpha$). *For given $U > 2\alpha > 0$, $N^{-1} E_U^{(N)}(\alpha)$ is bounded independently of N.*

Our lower bound on $N^{-1} E_U^{(N)}(\alpha)$ goes to $-\infty$ as $U \searrow 2\alpha$, but we are not claiming that this reflects the true state of affairs. Whether $\lim_{N \to \infty} N^{-1} E_{2\alpha}^{(N)}(\alpha)$ is finite or not remains an *open problem*; see, however, the discussion of the strong coupling limit below.

For U in the range $2\alpha < U < U_c(\alpha)$, there are bound states of an undetermined nature. Does the system become a gas of bipolarons or does it coalesce into a true N-particle bound state? If the latter, does this state exhibit a periodic structure, thereby forming a super-crystal on top of the underlying lattice of atoms? This is perhaps the physically most interesting *open problem*.

1.1. **The strong coupling limit.** There is a non-linear differential-integral variational principle associated with the polaron problem, which gives the exact ground

state energy in the limit $\alpha \to \infty$. This variational problem was investigated in detail by Pekar [28]. Pekar and Tomasevich (PT) [29] generalized it to the bipolaron, and the extension to N-polarons obviously follows from [29].

The PT functional is the result of a variational calculation and therefore gives an upper bound to the ground state energy $E_U^{(N)}(\alpha)$. In order to compute $\langle \Psi, H_U^{(N)} \Psi \rangle$, one takes a Ψ of the form $\psi \otimes \Phi$ where $\psi \in L^2(\mathbb{R}^{3N})$, $\Phi \in \mathcal{F}$, and both ψ and Φ are normalized. For a given ψ it is easy to compute the optimum Φ, and one ends up with the functional

$$\mathcal{P}_U^{(N)}[\psi] := \sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} |\nabla_i \psi|^2 \, dX + U \sum_{i<j} \int_{\mathbb{R}^{3N}} \frac{|\psi(X)|^2}{|x_i - x_j|} \, dX$$
$$- \alpha \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\psi(x)\, \rho_\psi(y)}{|x - y|} \, dx\, dy \,, \tag{1.9}$$

where $dX = \prod_{k=1}^{N} dx_k$, and

$$\rho_\psi(x) = \sum_{i=1}^{N} \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \ldots, x, \ldots, x_N)|^2 \, dx_1 \cdots \widehat{dx_i} \cdots dx_N \tag{1.10}$$

with x at the i-th position, and $\widehat{dx_i}$ meaning that dx_i has to be omitted in the product $\prod_{k=1}^{N} dx_k$. The ground state energy is

$$\mathcal{E}_U^{(N)}(\alpha) = \inf \left\{ \mathcal{P}_U^{(N)}[\psi] : \int_{\mathbb{R}^{3N}} |\psi|^2 \, dX = 1 \right\} . \tag{1.11}$$

Hence the variational argument above gives the upper bound

$$E_U^{(N)}(\alpha) \le \mathcal{E}_U^{(N)}(\alpha) = \mathcal{E}_{U/\alpha}^{(N)}(1) \, \alpha^2 \,. \tag{1.12}$$

(The equality follows by scaling.) For $N = 1$ this upper bound is due to Pekar; numerically, one has $\mathcal{E}^{(1)}(\alpha) \approx -(0.109)\alpha^2$ [25]. Moreover, the minimization problem for $\mathcal{E}^{(1)}(\alpha)$ has a unique minimizer (up to translations), see [18].

The upper bound for $N = 1$ was widely understood to be asymptotically exact for large α. A proof of this was finally achieved by Donsker and Varadhan [6], using large deviation theory applied to the functional integral discussed below. Later, this fact was rederived in [23] by operator methods, and it was shown that the error was no worse than $\alpha^{9/5}$ for large α.

The fact that for fixed ratio $\nu = U/\alpha \ge 0$

$$\lim_{\alpha \to \infty} \alpha^{-2} E_U^{(N)}(\alpha) = \mathcal{E}_\nu^{(N)}(\alpha = 1) \tag{1.13}$$

for $N = 2$ and any $\nu \ge 0$ was first noted in [26]. This is also valid for arbitrary N.

It follows from the limiting relation (1.13), together with the fact that our bound on $U_c(\alpha)$ is linear for large α, that our three theorems about $E_U^{(N)}(\alpha)$ transfer to the same theorems about $\mathcal{E}_U^{(N)}(\alpha)$ which we state next.

Corollary 1 (Stability and absence of binding for the PT functional).
1. Stability holds for $U > 2\alpha$, that is, for any $\nu > 2$ there is a constant $C(\nu)$ such that

$$\mathcal{E}_U^{(N)}(\alpha) \ge -C(\nu)\alpha^2 N \quad \text{for all } N \ge 2 \tag{1.14}$$

whenever $U = \nu\alpha > 0$.

2. There is no binding if U/α is large enough, that is, there is a finite $\nu_c > 2$ such that

$$\mathcal{E}_U^{(N)}(\alpha) = N\mathcal{E}^{(1)}(\alpha) \quad \text{for all } N \geq 2 \tag{1.15}$$

whenever $U \geq \nu_c\alpha$.

We note in passing that the critical U in the PT model depends linearly on α. This follows by scaling.

In Section 5 we will give a direct and easier proof of Corollary 1 that has no need of the functional integral machinery and leads to better constants. In particular, with our new proof we find that

$$C(\nu) \leq \begin{cases} (0.0280)\nu^3/(\nu - 2) & \text{if } 2 < \nu < 3\,, \\ 0.755 & \text{if } \nu \geq 3\,. \end{cases} \tag{1.16}$$

For fermions, a stronger result than Corollary 1 was obtained in [13]. They prove that at critical coupling $U = 2\alpha$ one has

$$\mathcal{E}_{2\alpha}^{(N)}(\alpha, q) \geq -(0.461)^2\alpha^2 q^{2/3}N \quad \text{for all } N \geq 2 \text{ and all } 1 \leq q \leq N\,, \tag{1.17}$$

where $\mathcal{E}_U^{(N)}(\alpha, q)$ is the infimum of $\mathcal{P}_U^{(N)}[\psi]$ restricted to fermions with q spin states ($q = 2$ for electrons). Recall that the single polaron energy is $\mathcal{E}^{(1)}(\alpha) = -(0.109)\alpha^2$ [25]. For completeness we repeat the short proof of (1.17) in Section 5.

1.2. **Previous results on the polaron ground state energy.** In addition to the large α asymptotics just mentioned, there have been several other rigorous results on the ground state energy of the (single) polaron, some of which we will use here.

(i) One of the earliest results was the variational calculation of $E^{(1)}(\alpha)$ for small α by Gurari and by Lee, Low, and Pines [14, 16, 17] which leads to

$$E^{(1)}(\alpha) \leq -\alpha \qquad \text{for all } \alpha\,. \tag{1.18}$$

(ii) A lower bound, which validates the conclusion that $E^{(1)}(\alpha) \sim -\alpha$ as $\alpha \to 0$, was obtained in [24]. They prove that

$$E^{(1)}(\alpha) \geq -\alpha - \frac{1}{3}\alpha^2 \qquad \text{for all } \alpha\,. \tag{1.19}$$

(To derive (1.19) use $p = 1 + 2\alpha/3$ in [24, Eq. (24)].) We note the fact that (1.19) has the correct power law behavior for both small and large α.

(iii) *The functional integral formulation*: The large time behavior of the heat kernel $\exp(-TH_U^{(N)})$ gives us the ground state energy as

$$E_U^{(N)}(\alpha) = -\lim_{T \to \infty} T^{-1}\ln\left\langle\exp\left(-TH_U^{(N)}\right)\right\rangle, \tag{1.20}$$

where $\langle\,\cdot\,\rangle$ denotes the expectation in a suitable state, i.e., a normalized vector in the Hilbert space. Since the phonon operators can be realized as the coordinates of a quantum-mechanical harmonic oscillator (one for each value of k), we can apply the Feynman-Kac formula for the evaluation of $\langle\exp(-TH_U^{(N)})\rangle$. Since the harmonic oscillator coordinates appear only linearly and quadratically in the exponent, they can then be integrated out

explicitly. One obtains a formula due to Feynman [7], see also [30, Sec. 5.3] for a careful discussion. The conclusion is that

$$E_U^{(N)}(\alpha) = -\lim_{R\to\infty}\lim_{T\to\infty} T^{-1}\ln Z_{U,R}^{(N)}(T)\,, \tag{1.21}$$

where

$$Z_{U,R}^{(N)}(T) := \int_{B_R} dx_1 \cdots \int_{B_R} dx_N \int dW_{x_1}^T(\omega_1)\cdots dW_{x_N}^T(\omega_N)\chi_{B_R}(\omega_1)\cdots\chi_{B_R}(\omega_N)$$

$$\times \exp\left(\alpha \int_{\mathbb{R}} \frac{ds\, e^{-|s|}}{2} \sum_{i,j=1}^N \int_0^T \frac{dt}{|\omega_i(t) - \omega_j(t+s)|}\right)$$

$$\times \exp\left(-U\sum_{i<j}\int_0^T \frac{dt}{|\omega_i(t)-\omega_j(t)|}\right)\,. \tag{1.22}$$

Here dW_x^T denotes the Wiener measure of closed Brownian paths in $\mathbb{R}^3$ with period T starting and ending at x. Moreover, B_R denotes the ball centered at the origin of radius R, and the characteristic function of the path $\chi_{B_R}(\omega_j)$ is 1 if ω_j stays inside the ball B_R for all times, and zero otherwise. The argument of $\omega_j(t+s)$ is understood modulo T.

2. THE TWO-POLARON PROBLEM: ABSENCE OF BINDING

We first consider the special case $N = 2$ and prove Theorem 2. It is convenient to structure the proof in three steps.

Step 1. Partition of the interparticle distance. We choose a quadratic partition of unity (IMS localization [4, Thm 3.2]) and localize the particles according to their *relative distance.* (In the N-particle case later on, we will localize with respect to the nearest neighbor distance, which, for $N = 2$, is the same as the relative distance.) This kind of localization is one of the principal novel features of our analysis.

In order to construct this partition, we pick some parameters $b > 1$ and $\ell > 0$, and let

$$\varphi(t) := \begin{cases} 0 & \text{for } t \leq \ell/b\,, \\ \sin\frac{\pi}{2}\frac{t-\ell/b}{\ell-\ell/b} & \text{for } \ell/b \leq t \leq \ell\,, \\ \cos\frac{\pi}{2}\frac{t-\ell}{b\ell-\ell} & \text{for } \ell \leq t \leq b\ell\,, \\ 0 & \text{for } t \geq b\ell\,. \end{cases} \tag{2.1}$$

For $j \geq 1$, let $\varphi_j(t) := \varphi(b^{1-j}t)$, and for $j = 0$, let

$$\varphi_0(t) := \begin{cases} 1 & \text{for } t \leq \ell/b\,, \\ \cos\frac{\pi}{2}\frac{t-\ell/b}{\ell-\ell/b} & \text{for } \ell/b \leq t \leq \ell\,, \\ 0 & \text{for } t \geq \ell\,. \end{cases} \tag{2.2}$$

Then

$$\sum_{j\geq 0}\varphi_j(t)^2 = 1 \quad \text{for all } t \geq 0\,. \tag{2.3}$$

Using the IMS localization formula, we can write, for any wave function ψ,

$$\langle\psi|H_U^{(2)}|\psi\rangle = \sum_{j\geq 0}\left\langle\psi_j\left|H_U^{(2)} - 2\sum_{k\geq 0}|\varphi_k'(|x_1 - x_2|)|^2\right|\psi_j\right\rangle =: \sum_{j\geq 0}e_j\|\psi_j\|^2 \tag{2.4}$$

with $\psi_j(x_1, x_2) = \psi(x_1, x_2)\varphi_j(|x_1 - x_2|)$ and with numbers e_j (depending on ψ_j). Our goal is to prove that $e_j \geq 2E^{(1)}(\alpha)$ for all j if $U \geq 2C\alpha$. If this is indeed the case, then the right side of (2.4) exceeds $2E^{(1)}(\alpha)\sum_j \|\psi_j\|^2 = 2E^{(1)}(\alpha)\|\psi\|^2$, which is the assertion of the theorem.

For our bounds we shall use the fact that on the support of $\varphi_j(|x_1 - x_2|)$, the localization error is dominated by

$$\sum_{k\geq 0}|\varphi_k'(|x_1 - x_2|)|^2 \leq \frac{\pi^2}{4(\ell - \ell/b)^2} \times \left\{ \begin{array}{ll} 1 & \text{if } j = 0\,, \\ b^{2(1-j)} & \text{if } j \geq 1\,. \end{array} \right. \tag{2.5}$$

Moreover, on these supports, we shall bound the Coulomb repulsion from below by

$$\frac{U}{|x_1 - x_2|} \geq b^{-j}\frac{U}{\ell} \qquad \text{for all } j \geq 0\,. \tag{2.6}$$

It is clear from (2.5) and (2.6) that by choosing U large enough, we can dominate the negative localization error by a part of the positive Coulomb term. What remains is to dominate the polaronic attraction by the remainder of the Coulomb repulsion. For this, we distinguish between the cases $j \geq 1$ and $j = 0$.

Step 2. The case $j \geq 1$; Energy estimate for separated particles. We further localize each of the two particles to its own ball of radius $b^j L$ for some parameter $L > 0$. This will entail an additional localization error. Concretely, let

$$\chi(x) = \frac{1}{\sqrt{2\pi}|x|}\left\{ \begin{array}{ll} \sin(\pi|x|) & \text{for } |x| \leq 1\,, \\ 0 & \text{for } |x| \geq 1\,, \end{array} \right. \tag{2.7}$$

and note that $\int dx\, \chi(x)^2 = 1$ and $\int dx |\nabla\chi(x)|^2 = \pi^2$. With

$$\psi_{j,u_1,u_2}(x_1, x_2) = \psi_j(x_1, x_2)(b^j L)^{-3}\chi(b^{-j}(x_1 - u_1)/L)\chi(b^{-j}(x_2 - u_2)/L) \tag{2.8}$$

we have, by a continuous version of the IMS localization formula,

$$\left\langle \psi_j \left| H_U^{(2)} - 2\sum_{k\geq 0}|\varphi_k'(|x_1 - x_2|)|^2 \right| \psi_j \right\rangle$$

$$= \int_{\mathbb{R}^3} du_1 \int_{\mathbb{R}^3} du_2 \left\langle \psi_{j,u_1,u_2} \left| H_U^{(2)} - 2\sum_{k\geq 0}|\varphi_k'(|x_1 - x_2|)|^2 - \frac{2\|\nabla\chi\|^2}{b^{2j}L^2} \right| \psi_{j,u_1,u_2} \right\rangle$$

$$\geq \int_{\mathbb{R}^3} du_1 \int_{\mathbb{R}^3} du_2 \left\langle \psi_{j,u_1,u_2} \left| H_U^{(2)} - b^{-2j}\left(\frac{b^2\pi^2}{2(\ell - \ell/b)^2} + \frac{2\pi^2}{L^2} \right) \right| \psi_{j,u_1,u_2} \right\rangle. \tag{2.9}$$

The latter inequality comes from (2.5). Note that since $|x_1 - x_2| \geq b^{j-2}\ell$ on the support of φ_j, the wave function ψ_{j,u_1,u_2} is non-zero only if the two balls of radius $b^j L$ centered at u_1 and u_2, respectively, are separated at least a distance

$$d \geq b^{j-2}\ell - 4b^j L\,. \tag{2.10}$$

We choose this to be positive by requiring that $L < \ell/(4b^2)$.

Lemma 1. *Assume that ψ is normalized and supported in $B_1 \times B_2$ where B_1 and B_2 are disjoint balls of some radius R, separated a distance d. Then*

$$\langle \psi | H_0^{(2)} | \psi \rangle \geq 2E^{(1)}(\alpha) - \frac{2\alpha}{d} \tag{2.11}$$

This lemma will be proved in Subsection 2.1. It is an easy consequence of the functional integral representation of the ground state energy.

We apply inequality (2.11) to (2.9). Using the bounds (2.10) on d and (2.6) on the Coulomb potential, we conclude that e_j is bounded from below as

$$e_j \geq 2E^{(1)}(\alpha) - b^{-j}\frac{2\alpha}{\ell/b^2 - 4L} + b^{-j}\frac{U}{\ell} - b^{-2j}\left(\frac{b^2\pi^2}{2(\ell - \ell/b)^2} + \frac{2\pi^2}{L^2}\right). \qquad (2.12)$$

This last expression is $\geq 2E^{(1)}(\alpha)$ for all $j \geq 1$ if and only if

$$\boxed{U \geq \frac{2\alpha\ell}{\ell/b^2 - 4L} + \frac{b\ell\pi^2}{2(\ell - \ell/b)^2} + \frac{2\pi^2\ell}{L^2 b}} \qquad \text{(the } j \geq 1 \text{ condition)}. \qquad (2.13)$$

Step 3. The case $j = 0$; Energy estimate for neighboring particles. Because of (2.5) and (2.6) we have the lower bound

$$e_0 \geq E_0^{(2)}(\alpha) - \frac{\pi^2}{2(\ell - \ell/b)^2} + \frac{U}{\ell}, \qquad (2.14)$$

where $E_0^{(2)}(\alpha)$ denotes the two-polaron energy in the absence of Coulomb repulsion, i.e., for $U = 0$. The following lemma compares this energy with $2E^{(1)}(\alpha)$.

Lemma 2. *For all $\alpha > 0$,*

$$E_0^{(2)}(\alpha) \geq 2E^{(1)}(\alpha) - \frac{7}{3}\alpha^2. \qquad (2.15)$$

Also this lemma uses the path integral formulation and we defer the proof to Subsection 2.1. At this point we will utilize it to conclude the proof of Theorem 2. The constant $7/3$ in (2.15) is certainly not optimal, and an improvement would lead to a better constant in Theorem 2.

It follows from (2.14) and (2.15) that $e_0 \geq 2E^{(1)}(\alpha)$ if

$$\boxed{U \geq \frac{7}{3}\ell\alpha^2 + \frac{\pi^2\ell}{2(\ell - \ell/b)^2}} \qquad \text{(the } j = 0 \text{ condition)}. \qquad (2.16)$$

Numerical evaluation shows that the two conditions (2.13) and (2.16) on U can be satisfied for an appropriate choice of b, ℓ, and L if $U \geq 61\,\alpha$. (Choose $b = 1.2$, $\ell = 22.8\,\alpha^{-1}$ and $L = 0.142\,\ell$.) For U satisfying these conditions, each $e_j \geq 2E^{(1)}(\alpha)$. This completes the proof of Theorem 2 with the bound on the constant $C < 30.5$. $\qquad\square$

In order to improve the bound on the constant C of Theorem 2, we replace Lemma 1 by the following alternative bound.

Lemma 3. *Under the same assumptions as in Lemma 1,*

$$\langle\psi|H_0^{(2)}|\psi\rangle \geq 2E^{(1)}(\alpha) - \left\langle\psi\left|\frac{2\alpha}{|x_1 - x_2|}\right|\psi\right\rangle - \frac{16\alpha R}{\pi^2 d(d + 4R)}. \qquad (2.17)$$

In the appendix we provide a proof of this lemma using the Rayleigh-Ritz variational principle. The proof is certainly not easier than the one of Lemma 1 using the functional integral method, but it may be of use in other applications where a functional integral approach is not as convenient (or available). The method does point up the utility of localizing the phonon field about the respective particles – in this case, to half-spaces each containing a particle.

We apply the bound (2.17) to (2.9), with $R = b^j L$ and d satisfying (2.10), and conclude that

$$e_j \geq 2E^{(1)}(\alpha) + b^{-j}\frac{U - 2\alpha}{\ell} - b^{-j}\frac{16\alpha Lb^2}{\ell\pi^2(\ell/b^2 - 4L)} - b^{-2j}\left(\frac{b^2\pi^2}{2(\ell - \ell/b)^2} + \frac{2\pi^2}{L^2}\right).$$
(2.18)

This expression is $\geq 2E^{(1)}(\alpha)$ for all $j \geq 1$ if and only if

$$\boxed{U \geq 2\alpha + \frac{16\alpha Lb^2}{\pi^2(\ell/b^2 - 4L)} + \frac{b\ell\pi^2}{2(\ell - \ell/b)^2} + \frac{2\pi^2\ell}{L^2b}}$$
(2.19)

Eqs. (2.16) and (2.19) are satisfied for $U \geq 53.2\,\alpha$ with the choice $b = 1.23$, $\ell = 19.7\,\alpha^{-1}$ and $L = 0.15\,\ell$.

2.1. **Some uses of the path integral.** Lemmas 1 and 2, used in the previous subsection, will be proved here.

Proof of Lemma 1. We use a Feynman-Kac representation similar to (1.21). It implies that the infimum of the left side of (2.11) over all ψ with the required support properties equals

$$-\lim_{T\to\infty}\frac{1}{T}\ln Z_{B_1,B_2}(T)$$
(2.20)

where

$$Z_{B_1,B_2}(T) := \int_{B_1} dx_1 \int_{B_2} dx_2 \int dW_{x_1}^T(\omega_1)dW_{x_1}^T(\omega_2)\chi_{B_1}(\omega_1)\chi_{B_2}(\omega_2)$$

$$\times \exp\left(\alpha \int_{\mathbb{R}}\frac{ds\,e^{-|s|}}{2}\sum_{i,j=1}^2\int_0^T\frac{dt}{|\omega_i(t) - \omega_j(t+s)|}\right).$$
(2.21)

Here $dW_{x_j}^T$ denotes the Wiener measure of closed Brownian paths in $\mathbb{R}^3$ with period T starting and ending at x_j, and $\chi_{B_j}(\omega_j)$ is 1 if ω_j stays inside the ball B_j for all times, and zero otherwise. Since $|\omega_1(t) - \omega_2(t+s)| \geq d$ for all t and s we see that $Z_{B_1,B_2}(T)$ is bounded from above by

$$e^{2\alpha T/d}\prod_{j=1}^2\left(\int_{B_j} dx \int dW_x^T(\omega_j)\chi_{B_j}(\omega_j)\exp\left(\alpha\int_{\mathbb{R}}\frac{ds\,e^{-|s|}}{2}\int_0^T\frac{dt}{|\omega_j(t) - \omega_j(t+s)|}\right)\right).$$

Replacing $\chi_{B_j}(\omega_j)$ by its upper bound 1, we deduce inequality (2.11). $\qquad\square$

Proof of Lemma 2. Application of the Cauchy-Schwarz inequality in the path integral (1.22) yields

$$Z_{0,R}^{(2)}(T)^2 \leq \iint dW_R^T(\omega_1)dW_R^T(\omega_2)$$

$$\times \exp\left(2\alpha\int_{\mathbb{R}}\frac{ds\,e^{-|s|}}{2}\sum_{i=1}^2\int_0^T\frac{dt}{|\omega_i(t) - \omega_i(t+s)|}\right)$$

$$\times \iint dW_R^T(\omega_1)dW_R^T(\omega_2)$$

$$\times \exp\left(4\alpha\int_{\mathbb{R}}\frac{ds\,e^{-|s|}}{2}\int_0^T\frac{dt}{|\omega_1(t) - \omega_2(t+s)|}\right),$$
(2.22)

where $\int dW_R^T(\omega)$ is short for $\int_{B_R} dx \int dW_x^T(\omega) \chi_{B_R}(\omega)$. The first factor on the right side equals the square of

$$\int dW_R^T(\omega) \exp\left(2\alpha \int_{\mathbb{R}} \frac{ds\, e^{-|s|}}{2} \int_0^T \frac{dt}{|\omega(t) - \omega(t+s)|} \right), \qquad (2.23)$$

which, in turn, is the one-polaron expression with α replaced by 2α. Using Jensen's inequality, we bound the second factor from above by

$$\int_{\mathbb{R}} \frac{ds\, e^{-|s|}}{2} \iint dW_R^T(\omega_1) dW_R^T(\omega_2) \exp\left(4\alpha \int_0^T \frac{dt}{|\omega_1(t) - \omega_2(t+s)|} \right). \qquad (2.24)$$

Since closed Brownian paths are invariant under time reparametrization, the latter integral does not actually depend on s, and hence (2.24) equals

$$\iint dW_R^T(\omega_1) dW_R^T(\omega_2) \exp\left(4\alpha \int_0^T \frac{dt}{|\omega_1(t) - \omega_2(t)|} \right). \qquad (2.25)$$

This functional integral represents two particles in the ball B_R interacting via an attractive Coulomb potential $-4\alpha/|x_1 - x_2|$. This is like the positronium Hamiltonian whose ground state energy equals $-2\alpha^2$ in the limit $R \to \infty$. Summarizing, after taking the $T \to \infty$ limit we find that

$$E_0^{(2)}(\alpha) \geq E^{(1)}(2\alpha) - \alpha^2. \qquad (2.26)$$

To finish the proof, we use the bounds (1.18) and (1.19), which imply that

$$E^{(1)}(2\alpha) \geq 2E^{(1)}(\alpha) - \frac{4}{3}\alpha^2. \qquad (2.27)$$

This, together with (2.26), proves (2.15). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

3. The N-polaron problem: Thermodynamic Stability

We now consider the case of general N and prove Theorem 3. We start by localizing particles in balls in order to reduce the problem to a local one. We use the sliding technique introduced in [3] (see also [21]). Pick an even and real-valued function χ with compact support, normalized by $\int \chi^2 = 1$, and $\omega > 0$ large enough such that the function

$$f(x) = \frac{1}{|x|}\left(1 - e^{-\omega|x|}\chi * \chi(x) \right) \qquad (3.1)$$

is positive definite. (The symbol $*$ means convolution.) The existence of such an ω for smooth enough χ was shown in [3, Lemma 2.1]. For any operator-valued function $\rho(x)$,

$$\iint dx\, dy \left(\sum_{i=1}^N \delta(x - x_i) - \rho(x)^\dagger \right) f(x - y) \left(\sum_{i=1}^N \delta(y - x_i) - \rho(y) \right) \geq 0. \qquad (3.2)$$

We apply this to

$$\rho(x) = \frac{1}{(2\pi)^2\sqrt{2\alpha}} \int dk\, |k| e^{ikx} a(k) \qquad (3.3)$$

and obtain the bound

$$\sum_{1 \leq i < j \leq N} \frac{2\alpha}{|x_i - x_j|} - \sqrt{\alpha} \sum_{i=1}^N \phi(x_i) + H_f \geq -\alpha N\omega + 2\alpha \int_{\mathbb{R}^3} dz\, I_\omega(z). \qquad (3.4)$$

Here,

$$I_\omega(z) := \sum_{1 \le i < j \le N} \chi_z(x_i) \frac{e^{-\omega|x_i - x_j|}}{|x_i - x_j|} \chi_z(x_j)$$

$$- \frac{1}{2} \sum_{i=1}^N \chi_z(x_i) \int dy \frac{e^{-\omega|x_i - y|}}{|x_i - y|} \chi_z(y) \left(\rho(y) + \rho(y)^\dagger \right)$$

$$+ \frac{1}{2} \iint dx \, dy \, \chi_z(x) \rho(x)^\dagger \frac{e^{-\omega|x - y|}}{|x - y|} \rho(y) \chi_z(y) \tag{3.5}$$

where we denote $\chi_z(x) = \chi(x - z)$. We also note that

$$p^2 = \int dz \, p \chi_z^2 p = \int dz \, \chi_z p^2 \chi_z - \int dx \, |\nabla\chi(x)|^2, \tag{3.6}$$

and thus

$$H_U^{(N)} \ge \int dz \, H_z + (U - 2\alpha) \, V_C - \alpha N \omega - \frac{N}{2} \int dx \, |\nabla\chi(x)|^2 \tag{3.7}$$

where

$$H_z := \frac{1}{2} \sum_{i=1}^N \left(\chi_z(x_i) p_i^2 \chi_z(x_i) + p_i \chi_z(x_i)^2 p_i \right) + 2\alpha \, I_\omega(z). \tag{3.8}$$

The Hamiltonian H_z is concerned only with the particles in the support of χ_z; similarly for the phonon field, $\rho(y)$ enters only for y in this support. Moreover, H_z commutes with $n_z = \sum_{i=1}^N \theta_z(x_i)$, the number of particles in the support of χ_z, where θ_z denotes the characteristic function of the support of χ_z. We can thus look for a lower bound on H_z in a fixed sector of n_z particles. We will prove the following lower bound.

Lemma 4. *With* $[t]_+ = \max\{t, 0\}$,

$$H_z \ge -\alpha \, [4\alpha n_z - \omega]_+ \sum_{i=1}^N \chi_z(x_i)^2 - \frac{3\alpha n_z}{(2\pi)^4} \left(\sqrt{\frac{2\pi}{3\omega}} \|\chi\|_\infty + \|\nabla\chi\|_2 \right)^2. \tag{3.9}$$

Proof. Pick some $\Lambda \ge \omega$. Applying (3.2) with the positive definite function $f(x) = |x|^{-1}(e^{-\omega|x|} - e^{-\Lambda|x|})$, we have

$$I_\omega(z) \ge I_\Lambda(z) - \frac{1}{2} (\Lambda - \omega) \sum_{i=1}^N \chi_z(x_i)^2. \tag{3.10}$$

The last term represent the 'self-energy' terms. We will choose Λ proportional to n_z, hence this term is of the order n_z^2. For the remaining terms, we complete the square and write

$$\chi_z(x_i) p_i^2 \chi_z(x_i) + p_i \chi_z(x_i)^2 p_i - 2\alpha \chi_z(x_i) \int dy \frac{e^{-\Lambda|x_i - y|}}{|x_i - y|} \chi_z(y) \left(\rho(y) + \rho(y)^\dagger \right)$$

$$= (\chi_z(x_i) p_i - A_z(x_i)) \left(p_i \chi_z(x_i) - A_z(x_i)^\dagger \right)$$

$$+ \left(p_i \chi_z(x_i) + A_z(x_i)^\dagger \right) (\chi_z(x_i) p_i + A_z(x_i))$$

$$- 2 A_z(x_i)^\dagger A_z(x_i) - \left[A_z(x_i), A_z(x_i)^\dagger \right], \tag{3.11}$$

where $A_z(x)$ is a vector operator with three components,

$$A_z(x) := \frac{\alpha}{\pi^2} \int dy \, \chi_z(y)\rho(y) \int dk \frac{k \, e^{ik(y-x)}}{k^2 \, (k^2 + \Lambda^2)} \,. \tag{3.12}$$

The Schwarz inequality applied to this last equation shows that

$$A_z(x)^\dagger A_z(x) \leq \int dw \, dy \, \chi_z(w)\rho(w)^\dagger \frac{e^{-\Lambda|w-y|}}{|w-y|} \rho(y)\chi_z(y) \, \frac{2\alpha^2}{\pi^2} \int dk \frac{1}{k^2(k^2 + \Lambda^2)} \,. \tag{3.13}$$

Moreover,

$$[A_z(x), A_z(x)^\dagger] = \frac{2\alpha}{(2\pi)^4} \sum_{i=1}^{3} \int |\nabla_y \left(\chi_z(y)f_i(\Lambda(x-y))\right)|^2 \, dy$$

$$\leq \frac{2\alpha}{(2\pi)^4} \sum_{i=1}^{3} \left(\Lambda^{-1/2}\|\chi\|_\infty\|\nabla f_i\|_2 + \|\nabla\chi\|_2\|f_i\|_\infty\right)^2 \tag{3.14}$$

with

$$f_i(x) = \frac{x_i}{|x|} \frac{1 - (1 + |x|)e^{-|x|}}{|x|^2} \quad, \quad x = (x_1, x_2, x_3) \,. \tag{3.15}$$

We choose Λ such that

$$n_z \frac{2\alpha^2}{\pi^2} \int dk \frac{1}{k^2(k^2 + \Lambda^2)} = \frac{4\alpha^2 n_z}{\Lambda} \leq \alpha \,, \tag{3.16}$$

which then assures that the last two terms of equation (3.11) are relatively bounded by the field energy terms, i.e., the last term of $I_\omega(z)$ in (3.5). More precisely, with the choice $\Lambda = \max\{\omega, 4\alpha n_z\}$ Lemma 4 follows, using the facts $\|f_i\|_\infty = 1$, $\|\nabla f_i\|_2^2 = 2\pi/3$, and the commutator bound (3.14), this bound contributing the last term on the right side of (3.9). $\square$

We now complete the proof of Theorem 3. If we insert bound (3.9) into (3.7), we obtain the following lower bound on $H_U^{(N)}$:

$$H_U^{(N)} \geq -\alpha \int dz \left(\omega + [4\alpha n_z - \omega]_+\right) \sum_{i=1}^{N} \chi_z(x_i)^2 + (U - 2\alpha) V_C$$

$$- \frac{N}{2} \int dx \, |\nabla\chi(x)|^2 - \frac{3\alpha}{(2\pi)^4} N \, |\text{supp} \, \chi| \left(\sqrt{\frac{2\pi}{3\omega}}\|\chi\|_\infty + \|\nabla\chi\|_2\right)^2 . \tag{3.17}$$

The volume of the support of χ, $|\text{supp} \, \chi| = \int \theta_0$, enters via the identity $\int dz \, n_z = N|\text{supp} \, \chi|$. We further bound $[4\alpha n_z - \omega]_+ \leq 4\alpha n_z$, and use that

$$\int dz \, n_z \sum_{i=1}^{N} \chi_z(x_i)^2 = \sum_{i,j=1}^{N} \int dz \, \theta_z(x_j)\chi_z(x_i)^2$$

$$= 2 \sum_{1 \leq i < j \leq N} \int dz \, \theta_z(x_j)\chi_z(x_i)^2 + N \,. \tag{3.18}$$

Moreover,

$$\int dz \, \theta_z(x_j)\chi_z(x_i)^2 \leq \frac{Z}{|x_i - x_j|} \tag{3.19}$$

with

$$Z := \sup_{x \in \mathbb{R}^3} |x| \left(\theta_0 * \chi^2 \right)(x). \tag{3.20}$$

The final result is

$$H_U^{(N)} \geq \left(U - 2\alpha - 8\alpha^2 Z \right) V_C - 4\alpha^2 N - \alpha N \omega$$

$$- \frac{N}{2} \|\nabla \chi\|_2^2 - \frac{3\alpha}{(2\pi)^4} N \, |\text{supp} \, \chi| \left(\sqrt{\frac{2\pi}{3\omega}} \|\chi\|_\infty + \|\nabla \chi\|_2 \right)^2. \tag{3.21}$$

Note that Z is bounded above by the diameter of the support of χ, which can be chosen arbitrarily small. In particular, we can choose the diameter small enough such that $8\alpha^2 Z \leq U - 2\alpha$, which leads to a lower bound on $H_U^{(N)}$ that is linear in N. This concludes the proof of Theorem 3. $\qquad \square$

For $U = \nu\alpha$, $\nu > 2$, our lower bound is proportional to $\alpha^2 N$ for large α. To see this, we choose the diameter of the support of χ to be of the order $1/\alpha$. Hence $Z \sim \alpha^{-1}$, and also $\omega \sim \alpha$ by scaling. Moreover, $\|\nabla \chi\|_2 \sim \alpha$, $\|\chi\|_\infty \sim \alpha^{3/2}$ and $|\text{supp} \, \chi| \sim \alpha^{-3}$, hence the right side of (3.21) is of the desired form, namely, $- \text{const} \, \alpha^2 N$ for large α.

We conjecture that, for $U = \nu\alpha$, $\nu > 2$,

$$H_U^{(N)} \geq N E^{(1)}(\alpha) - C_\nu N \alpha^2 \quad \text{for all } \alpha > 0, \tag{3.22}$$

for some constant C_ν depending only on ν. For $N = 2$ this was proved in the previous section, but the proof of (3.22) for general $N \geq 2$ remains an *open problem*.

4. The N-polaron problem: Absence of Binding

We now return to the question of binding of polarons and prove Theorem 1. Because of subadditivity of the energy (1.8), $E_U^{(N)}(\alpha) \leq N E^{(1)}(\alpha)$ for any N, U and α. Hence it remains to prove the reverse inequality.

We perform a localization similar to that in the two-polaron case, but *relative to the nearest neighbor*. This type of localization is one of the main technical ingredients in our proof. As in the bipolaron case, the goal will be to localize each particle in a box whose size is of the same order as the distance to the closest particles, as long as this distance is not too small.

Let φ_i be given as in (2.1)–(2.2), for some $\ell > 0$ and $b > 1$. If t_i denotes the distance of x_i to the nearest neighbor among the x_j, $j \neq i$, then

$$1 = \sum_{j_1, \ldots, j_N} \prod_{i=1}^{N} |\varphi_{j_i}(t_i)|^2 \tag{4.1}$$

and, by the IMS localization formula,

$$\langle \psi | H_U^{(N)} | \psi \rangle$$

$$= \sum_{j_1, \ldots, j_N} \left\langle \psi \prod_i \varphi_{j_i}(t_i) \, \middle| \, H_U^{(N)} - \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_k |\nabla_i \varphi_k(t_j)|^2 \, \middle| \, \psi \prod_i \varphi_{j_i}(t_i) \right\rangle. \tag{4.2}$$

We claim that the following bound on the localization error holds.

Lemma 5. *On the support of* $\varphi_{j_i}(t_i)$,

$$\sum_{j=1}^{N} \sum_{k} |\nabla_i \varphi_k(t_j)|^2 \leq \frac{\gamma}{(\ell - \ell/b)^2} b^{2(1-j_i)} \tag{4.3}$$

with $\gamma := 13(\pi/2)^2$.

Proof. Note that $\varphi_k(t_j)$ depends on x_i in one of two ways. First, through t_i when $j = i$, but also through all the t_j, $j \neq i$, where x_i happens to be the nearest neighbor of x_j.

We claim that there can be at most 12 of those x_j. If x is the nearest neighbor of both x_j and x_k, then $|x_j - x_k| \geq \max\{|x_j - x|, |x_k - x|\}$, and hence the angle between $x_j - x$ and $x_k - x$ is at least $\pi/3$. Think of x as the center of a unit sphere. The lines from x to each of these x_j's intersects the unit sphere at certain points p_j, whose angular separation is at least $\pi/3$. At each of these points p_j we can, therefore, construct a unit sphere tangent at p_j to the given sphere around x. From the packing problem we know there can be at most 12 such spheres. This proves the claim.

On the support of $\varphi_{j_i}(t_i)$,

$$\sum_{k} |\nabla_i \varphi_k(t_i)|^2 \leq \frac{\pi^2}{4(\ell - \ell/b)^2} b^{2(1-j_i)} \tag{4.4}$$

as we have already used in (2.5). If x_i is the nearest neighbor of x_j, the same is true with t_i replaced by t_j on the left side, since $t_j \geq t_i$ by definition, and the left side is easily seen to be decreasing in t_i. This concludes the proof. $\square$

We now proceed with the one-particle localization as in the two-polaron case, localizing particle i in a ball of radius $b^{j_i} L$ centered at u_i, with $L < \ell/(4b^2)$. More precisely, with χ given in (2.7), let

$$\psi_{\mathbf{j},\mathbf{u}}(X) = \psi(X) \prod_{i=1}^{N} \left[\varphi_{j_i}(t_i)(b^{j_i} L)^{-3/2} \chi(b^{-j_i}(x_i - u_i)/L) \right] \tag{4.5}$$

where $\mathbf{j} = (j_1, \ldots, j_N)$ and $\mathbf{u} = (u_1, \ldots, u_N)$. We have

$$\|\psi\|^2 = \sum_{\mathbf{j}} \int_{\mathbb{R}^{3N}} d\mathbf{u} \, \|\psi_{\mathbf{j},\mathbf{u}}\|^2 \tag{4.6}$$

and, using Lemma 5,

$$\langle \psi | H_U^{(N)} | \psi \rangle$$

$$= \sum_{\mathbf{j}} \int_{\mathbb{R}^{3N}} d\mathbf{u} \left\langle \psi_{\mathbf{j},\mathbf{u}} \left| H_U^{(N)} - \sum_{i=1}^{N} \left(\sum_{k_1,\ldots,k_N} \left| \nabla_i \prod_j \varphi_{k_j}(t_j) \right|^2 + \frac{\|\nabla \chi\|_2^2}{b^{2j_i} L^2} | \right) \right| \psi_{\mathbf{j},\mathbf{u}} \right\rangle$$

$$\geq \sum_{\mathbf{j}} \int_{\mathbb{R}^{3N}} d\mathbf{u} \left\langle \psi_{\mathbf{j},\mathbf{u}} \left| H_U^{(N)} - \sum_{i=1}^{N} b^{-2j_i} \left(\frac{\gamma b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} \right) \right| \psi_{\mathbf{j},\mathbf{u}} \right\rangle . \tag{4.7}$$

In analogy with the two-particle problem, the goal here is to show that the integrand in this last expression is bounded below by $N E^{(1)}(\alpha) \|\psi_{\mathbf{j},\mathbf{u}}\|^2$ which, together with (4.6), implies the conclusion of the theorem.

For given $\mathbf{j}$ and $\mathbf{u}$, let B_i denote the ball of radius $b^{j_i}L$ centered at u_i. Because of our assumption $L < \ell/(4b^2)$, the balls B_i with $j_i \geq 1$ do not intersect any of the other balls. Let d_{ik} denote the distance between ball B_i and ball B_k.

Recall that the ground state energy can be obtained from the $T \to \infty$ asymptotics of the functional integral (1.22). In the case of relevance here, for states having the aforementioned support properties of $\psi_{\mathbf{j},\mathbf{u}}$, the Brownian paths ω_i in the functional integral are confined to the respective balls B_i. In addition to this confinement, the paths have the property that at any given time t, the separation between any $\omega_i(t)$ and its nearest neighbor among the $\omega_k(t)$, $k \neq i$, satisfies the conditions according to the support of φ_{j_i}. We may relabel the particles such that $j_i = 0$ for $i \leq M$, and $j_i \geq 1$ for $M < i \leq N$. The exponential in the functional integral is a sum of three pieces, $\mathcal{A} + \mathcal{B} + \mathcal{C}$, where

$$\mathcal{A} = \sum_{k=M+1}^{N} \sum_{i=1}^{k-1} \left(2\alpha \int_{\mathbb{R}} \frac{ds\, e^{-|s|}}{2} \int_0^T \frac{dt}{|\omega_i(t) - \omega_k(t+s)|} - U \int_0^T \frac{dt}{|\omega_i(t) - \omega_k(t)|} \right),$$
(4.8)

$$\mathcal{B} = \sum_{k=M+1}^{N} \alpha \int_{\mathbb{R}} \frac{ds\, e^{-|s|}}{2} \int_0^T \frac{dt}{|\omega_i(t) - \omega_i(t+s)|},$$
(4.9)

and

$$\mathcal{C} = \alpha \sum_{i,k=1}^{M} \int_{\mathbb{R}} \frac{ds\, e^{-|s|}}{2} \int_0^T \frac{dt}{|\omega_i(t) - \omega_k(t+s)|} - U \sum_{1 \leq i < k \leq M} \int_0^T \frac{dt}{|\omega_i(t) - \omega_k(t)|}.$$
(4.10)

We first bound $\mathcal{A}$. For $k > M$ and $i \neq k$, the distance d_{ik} between the balls B_i and B_k is nonzero. Since the paths ω_i and ω_k are confined to the balls B_i and B_k, respectively,

$$\mathcal{A} \leq T \sum_{k=M+1}^{N} \sum_{i=1}^{k-1} \left(\frac{2\alpha}{d_{ik}} - \frac{U}{d_{ik} + 2L(b^{j_i} + b^{j_k})} \right).$$

Similar to (2.10),
$$d_{ik} \geq b^{\max\{j_i, j_k\}-2}\ell - 4b^{\max\{j_i, j_k\}}L,$$
(4.11)

and hence

$$\mathcal{A} \leq -T \left(U \left(1 - \frac{4Lb^2}{\ell} \right) - 2\alpha \right) \sum_{k=M+1}^{N} \sum_{i=1}^{k-1} \frac{1}{d_{ik}}.$$
(4.12)

Under the assumption that $U(1 - 4Lb^2/\ell) > 2\alpha$ this is negative. We not only want it to be negative, however, we also want it to dominate part of the localization error, namely,

$$\left(\frac{\gamma\, b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} \right) \sum_{k=M+1}^{N} b^{-2j_k}.$$

Using the fact that $\min_{i \neq k} d_{ik} \leq \ell b^{j_k} \leq \ell b^{2j_k-1}$ we can bound

$$\sum_{k=M+1}^{N} b^{-2j_k} \leq 2\ell b^{-1} \sum_{k=M+1}^{N} \sum_{i=1}^{k-1} \frac{1}{d_{ik}}.$$
(4.13)

From (4.12) and (4.13), we conclude that

$$\mathcal{A} + T \left(\frac{\gamma b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} \right) \sum_{k=M+1}^{N} b^{-2j_k} \leq 0 \qquad (4.14)$$

as long as

$$U \left(1 - \frac{4Lb^2}{\ell} \right) \geq 2\alpha + \frac{2\ell}{b} \left(\frac{\gamma b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} \right) . \qquad (4.15)$$

Since we are seeking a lower bound on the energy, i.e., an upper bound on the functional integral, (4.15) then implies that $\mathcal{A}$, together with the localization terms coming from $M < i \leq N$ in (4.7), are indeed negative by (4.14). Therefore these terms can be discarded in the functional integral. This concludes the discussion of the term $\mathcal{A}$ and leaves us with $\mathcal{B} + \mathcal{C}$ and the remaining localization terms from (4.7) corresponding to $1 \leq i \leq M$.

Since $\mathcal{B}$ and $\mathcal{C}$ refer to different, now non-interacting, sets of particles (namely, $M + 1 \leq k \leq N$ and $1 \leq i \leq M$), we see that the functional integral factorizes. The term $\mathcal{B}$ is just the exponent in the path integral for $(N - M)$ non-interacting polarons, each with its own field. The integral of $e^{\mathcal{B}}$ contributes $(N - M)E^{(1)}(\alpha)$ to the energy. Henceforth we can forget about $\mathcal{B}$.

With the aid of our previous linear lower bound for $U > 2\alpha$, term $\mathcal{C}$ is almost as simple as term $\mathcal{B}$. Since $U > 2\alpha$ we can write $U = 2\alpha + Z + V$ with Z and V, both positive, to be chosen later. Because of the separation condition for any $1 \leq i \leq M$ and any time t, the distance between $\omega_i(t)$ and its nearest neighbor among the $\omega_k(t)$'s is bounded above by ℓ, and hence

$$\sum_{1 \leq i < k \leq M} \frac{V}{|\omega_i(t) - \omega_k(t)|} \geq \frac{V}{\ell} M . \qquad (4.16)$$

The integral of $e^{\mathcal{C}}$ contributes at least

$$E_{2\alpha+Z}^{(M)}(\alpha) + M \frac{V}{\ell} \qquad (4.17)$$

to the energy. By Theorem 3 this is bounded from below by $-MC(2\alpha + Z, \alpha) + MV/\ell$, where $C(2\alpha + Z, \alpha)$ is the finite constant implicit in Theorem 3. This term is at least

$$ME^{(1)}(\alpha) + M \left(\frac{\gamma b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} \right)$$

(the second term being the localization error from (4.7)) provided we take

$$V = \ell \left(E^{(1)}(\alpha) + \frac{\gamma b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} + C(2\alpha + Z, \alpha) \right) . \qquad (4.18)$$

Another way to state this is that U must satisfy

$$U \geq 2\alpha + Z + \ell \left(\frac{\gamma b^2}{(\ell - \ell/b)^2} + \frac{\pi^2}{L^2} \right) + \ell \sup_{n \geq 2} \left| \frac{E_{2\alpha+Z}^{(n)}(\alpha)}{n} - E^{(1)}(\alpha) \right| \qquad (4.19)$$

for some $Z > 0$.

We have thus shown that, for any given $\mathbf{j}$ and $\mathbf{u}$, the integrand in the first line of (4.7) is bounded from below by $NE^{(1)}(\alpha)\|\psi_{\mathbf{j},\mathbf{u}}\|^2$ as long as U satisfies the bounds

(4.15) and (4.19) (for some $Z > 0$). In combination with (4.6), this concludes the proof of Theorem 1. □

There are many parameters in (4.15) and (4.19): b, ℓ, L and Z. The only constraint on them is $b > \ell > 4Lb^2$, and each choice gives rise to a computable estimate on the critical U. We emphasize that the resulting bound on U is independent of N.

Our bound on the critical value $U_c(\alpha)$ is proportional to α for large α. This follows with the choice $\ell \sim L \sim \alpha^{-1}$ and $b = O(1)$, in which case condition (4.15) is of the form $U \geq \text{const } \alpha$. With $Z \sim \alpha$, condition (4.19) is also of this form for large α, since the last term is bounded by const α^2 for large α, as shown in the previous section. We conjecture that the last term in (4.19) is actually bounded by α^2 for *all* α, as explained at the end of the previous section, Eq. (3.22). Assuming the validity of (3.22), our method leads to the bound $U_c(\alpha) \leq \text{const } \alpha$ for *all* $\alpha > 0$.

5. The Pekar-Tomasevich functional

5.1. **Boltzons for $U > 2\alpha$.** We shall prove the analogue of Theorem 3 for the PT functional. The designation 'boltzons' refers to particles without any symmetry restriction.

Proposition 1. *If $U > 2\alpha$ then*

$$\mathcal{E}_U^{(N)}(\alpha) \geq \begin{cases} -(0.0280)NU^3/(U - 2\alpha) & \text{if } 2\alpha < U < 3\alpha\,, \\ -(0.755)N\alpha^2 & \text{if } U \geq 3\alpha\,. \end{cases} \tag{5.1}$$

We note that this proves (1.14) with the constant stated in (1.16).

Proof. We write $U = 2(\alpha + \delta)$ with some $\delta > 0$. Given any ψ, and hence ρ_ψ, we will use two inequalities to bound the first two terms in the functional (1.9) in terms of ρ_ψ. The first is the Hoffmann-Ostenhof inequality [15] (see also [20, Cor. 8.4]),

$$\sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} |\nabla_i \psi(X)|^2 \, dX \geq \int_{\mathbb{R}^3} |\nabla \sqrt{\rho_\psi}(x)|^2 \, dx\,. \tag{5.2}$$

The second is the Lieb-Oxford inequality [19], [20, Thm. 6.1]

$$\sum_{i<j} \int_{\mathbb{R}^{3N}} \frac{|\psi(X)|^2}{|x_i - x_j|} \, dX \geq \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_\psi(x)\, \rho_\psi(y)}{|x - y|} \, dx \, dy - (1.68) \int_{\mathbb{R}^3} \rho_\psi(x)^{4/3} \, dx\,. \tag{5.3}$$

These two bounds imply that (with $\phi := \sqrt{\rho_\psi/N}$)

$$\frac{1}{N}\mathcal{P}_U^{(N)}[\psi] \geq \int_{\mathbb{R}^3} \left(|\nabla\phi|^2 - (1.68)UN^{1/3}\phi^{8/3} \right) dx + \delta N \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\phi(x)^2 \, \phi(y)^2}{|x - y|} \, dx \, dy\,. \tag{5.4}$$

Next, we use Hölder's inequality

$$\int \phi^{8/3} \, dx \leq \left(\int_{\mathbb{R}^3} \phi^3 \, dx \right)^{2/3} \left(\int_{\mathbb{R}^3} \phi^2 \, dx \right)^{1/3} \tag{5.5}$$

and Lemma 6 below to conclude that

$$\int \phi^{8/3} \, dx \leq \frac{1}{(4\pi)^{1/3}} \left(\iint \frac{\phi(x)^2 \, \phi(y)^2}{|x - y|} \, dx \, dy \right)^{1/3} \left(\int |\nabla\phi|^2 \, dx \right)^{1/3} \left(\int \phi^2 \, dx \right)^{1/3}. \tag{5.6}$$

Using $(\alpha\beta\gamma)^{1/3}abc \leq \frac{1}{3}(\alpha a^3 + \beta b^3 + \gamma c^3)$ for non-negative numbers $a, b, c, \alpha, \beta, \gamma$, we see that

$$(1.68)UN^{1/3}\int \phi^{8/3}\,dx \leq \int |\nabla\phi|^2\,dx + \delta N \iint \frac{\phi(x)^2\,\phi(y)^2}{|x-y|}\,dx\,dy$$
$$+ \frac{(1.68U)^3}{4\pi 3^3\delta}\int \phi^2\,dx\,. \tag{5.7}$$

This, together with (5.4) leads to the lower bound

$$\mathcal{E}_U^{(N)}(\alpha) \geq -\frac{(1.68)^3}{54\pi}\frac{U^3}{U-2\alpha}N\,. \tag{5.8}$$

While this is true for all $U > 2\alpha$, the right side is not a monotone increasing function of U, which we know the left side to be. Therefore we can say that $\mathcal{E}_U^{(N)}(\alpha)$ is bounded from below by the maximum value of the right side once U exceeds the maximum point, which is $U = 3\alpha$. This concludes the proof. $\qquad\square$

Lemma 6. *For non-negative functions ϕ*

$$\left(\int_{\mathbb{R}^3}\phi^3\,dx\right)^2 \leq \frac{1}{4\pi}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\phi(x)^2\,\phi(y)^2}{|x-y|}\,dx\,dy\,\int_{\mathbb{R}^3}|\nabla\phi(x)|^2dx\,. \tag{5.9}$$

Proof. We apply Schwarz's inequality

$$\left(\int_{\mathbb{R}^3}\phi^3\,dx\right)^2 = \langle |p|^{-1}\phi^2\,|\,|p|\phi\rangle^2 \leq \left\langle\phi^2\left|\frac{1}{p^2}\right|\phi^2\right\rangle\left\langle\phi\left|p^2\right|\phi\right\rangle \tag{5.10}$$

and recall that $|p|^{-2}$ is convolution with $(4\pi|x|)^{-1}$. $\qquad\square$

The stability of the PT functional with critical repulsion $U = 2\alpha$ remains an *open problem*. In the fermionic case the answer is affirmative, as was shown by Griesemer and Møller [13]. For the reader's convenience we include the proof here.

Combining the Lieb-Thirring inequality [22] [20, Cor. 4.1]

$$\sum_{i=1}^{N}\int_{\mathbb{R}^{3N}}|\nabla_i\psi(X)|^2\,dX \geq Kq^{-2/3}\int_{\mathbb{R}^3}\rho_\psi(x)^{5/3}\,dx\,. \tag{5.11}$$

where $K := \frac{9}{5}(2\pi)^{2/3} = 6.13$ [5], with the Lieb-Oxford inequality (5.3), one deduces

$$\mathcal{P}_{2\alpha}^{(N)}[\psi] \geq Kq^{-2/3}\int_{\mathbb{R}^3}\rho_\psi(x)^{5/3}\,dx - 2\alpha(1.68)\int_{\mathbb{R}^3}\rho_\psi(x)^{4/3}\,dx\,. \tag{5.12}$$

The minimization of the expression on the right side under the normalization constraint $\int_{\mathbb{R}^3}\rho_\psi(x)\,dx = N$ leads to the lower bound

$$\mathcal{P}_{2\alpha}^{(N)}[\psi] \geq -\frac{(1.68)^2}{K}q^{2/3}N\alpha^2\,, \tag{5.13}$$

as claimed in Eq. (1.17).

5.2. **Absence of binding in the Pekar-Tomasevich model.** We have just given an alternative proof of the fact that there is stability of matter in the PT model when $U > 2\alpha$. Now we discuss the other part of Corollary 1, that is, the absence of binding for large U.

The first step is to linearize the problem. The variational problem for the PT functional can, equivalently, be written

$$\mathcal{E}_U^{(N)}(\alpha) = \inf_{\psi,\sigma} \left\{ \left\langle \psi \left| \mathcal{H}_{U,\sigma}^{(N)} \right| \psi \right\rangle : \int_{\mathbb{R}^{3N}} |\psi|^2 \, dX = 1 \right\} \tag{5.14}$$

where the N-particle Hamiltonian $\mathcal{H}_{U,\sigma}^{(N)}$ is defined to be

$$\mathcal{H}_{U,\sigma}^{(N)} := \sum_{i=1}^{N} \left(-\Delta_i - 2\alpha \int_{\mathbb{R}^3} \frac{\sigma(y)}{|x_i - y|} \, dy \right) + U \sum_{i<j} \frac{1}{|x_i - x_j|}$$

$$+ \alpha \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\sigma(x) \, \sigma(y)}{|x - y|} \, dx \, dy. \tag{5.15}$$

We proceed as before, by localizing particles into individual boxes, with sizes depending on the distance to the nearest neighbor. In each localization region we obtain a lower bound on the energy of a given ψ by minimizing over σ, which yields the PT functional for the localized ψ. (In other words, we linearize, localize, and de-linearize. If we had not followed this route and tried to deal with the quartic term directly, the resulting expressions would be much more complicated.)

Consider first the case $N = 2$. In the region $j = 0$, we need a lower bound on $\mathcal{E}_0^{(2)}(\alpha)$. We could use Lemma 2 above, but it is simpler, and indeed more accurate, to use

$$\mathcal{E}_0^{(2)}(\alpha) = 2\,\mathcal{E}_0^{(1)}(2\alpha) = 8\,\mathcal{E}_0^{(1)}(\alpha) = 2\,\mathcal{E}_0^{(1)}(\alpha) - 6 \cdot (0.109)\,\alpha^2. \tag{5.16}$$

The first equality follows from the linearization (5.14) since the ground state of (5.15) for $U = 0$ is a product function for every σ; the second equality follows by scaling.

For the regions $j \geq 1$, we obtain the PT functional for 2 particles localized in disjoint balls. The proof of the corresponding lower bound to the energy, analogous to Lemma 1, is obvious, bounding the attractive energy using the smallest possible distance of the particles. Alternatively, one can use Lemma 3. For $j \geq 1$ the resulting condition on U is thus the same as in the proof of Theorem 2. Our improved estimate in the $j = 0$ region leads to the bound $\nu_c \leq 29.4$ (to be compared with the bound $C < 2 \cdot (26.6) = 53.2$ for the Fröhlich polaron).

We can similarly analyze the N-particle problem. For the particles with $j \geq 1$ the bounds are exactly the same as before, except that functional integrals are not needed in the derivation. For the particles with $j = 0$ the improved stability bound (5.1) (or (1.17) for fermions) is used, and hence the final condition for the absence of binding will be a lower value of U than that for the Fröhlich Hamiltonian. $\square$

Appendix A. Proof of Lemma 3

We assume that the confining balls B_1, B_2 are each of radius R, and that the balls are of distance $d = \inf\{|x_1 - x_2| : x_1 \in B_1, \ x_2 \in B_2\}$ from each other. In the

following, let

$$\hat{a}(x) = \frac{1}{(2\pi)^{3/2}} \int dk\, e^{ikx} a(k)\,, \ \hat{a}^\dagger(x) = \frac{1}{(2\pi)^{3/2}} \int dk\, e^{-ikx} a^\dagger(k) \tag{A.1}$$

be normalized annihilation and creation operators, with x a point in configuration space. In terms of these operators, the particle- field interaction term in $H_U^{(2)}$ is given by

$$\sqrt{\alpha}\phi(x) = \frac{\sqrt{\alpha}}{\pi^{3/2}} \int dy\, \frac{\hat{a}^\dagger(y) + \hat{a}(y)}{|x-y|^2} \tag{A.2}$$

and the phonon field energy by

$$H_f = \int dx\, \hat{a}^\dagger(x)\hat{a}(x). \tag{A.3}$$

Fix a plane midway between the two balls and perpendicular to the line between their centers, and let S_1 and S_2 be the resulting half-spaces with $B_1 \subset S_1$ and $B_2 \subset S_2$. Then we have the identity

$$\begin{aligned}
H_{U=0}^{(2)} = {}& p_1^2 - \frac{\sqrt{\alpha}}{\pi^{3/2}} \int_{S_1} dy\, \frac{\hat{a}^\dagger(y) + \hat{a}(y)}{|x_1-y|^2} \\
& + \int_{S_1} dy \left(\hat{a}^\dagger(y) - \frac{\sqrt{\alpha}}{\pi^{3/2}|x_2-y|^2} \right) \left(\hat{a}(y) - \frac{\sqrt{\alpha}}{\pi^{3/2}|x_2-y|^2} \right) \\
& + p_2^2 - \frac{\sqrt{\alpha}}{\pi^{3/2}} \int_{S_2} dy\, \frac{\hat{a}^\dagger(y) + \hat{a}(y)}{|x_2-y|^2} \\
& + \int_{S_2} dy \left(\hat{a}^\dagger(y) - \frac{\sqrt{\alpha}}{\pi^{3/2}|x_1-y|^2} \right) \left(\hat{a}(y) - \frac{\sqrt{\alpha}}{\pi^{3/2}|x_1-y|^2} \right) \\
& - \frac{\alpha}{\pi^3} \int_{S_1} \frac{dy}{|x_2-y|^4} - \frac{\alpha}{\pi^3} \int_{S_2} \frac{dy}{|x_1-y|^4}\,. \tag{A.4}
\end{aligned}$$

Define

$$\hat{a}_{x_2}(y) \equiv \left(\hat{a}(y) - \frac{\sqrt{\alpha}}{\pi^{3/2}|x_2-y|^2} \right),\ y \in S_1 \tag{A.5}$$

and analogous expressions for $\hat{a}_{x_2}^\dagger(y)$, and for $\hat{a}_{x_1}(y), \hat{a}_{x_1}^\dagger(y)$ with $y \in S_2$. In terms of these operators, the identity (A.4) becomes

$$\begin{aligned}
H_{U=0}^{(2)} = {}& p_1^2 - \frac{\sqrt{\alpha}}{\pi^{3/2}} \int_{S_1} dy\, \frac{\hat{a}_{x_2}^\dagger(y) + \hat{a}_{x_2}(y)}{|x_1-y|^2} + \int_{S_1} dy\, \hat{a}_{x_2}^\dagger(y)\hat{a}_{x_2}(y) \\
& + p_2^2 - \frac{\sqrt{\alpha}}{\pi^{3/2}} \int_{S_2} dy\, \frac{\hat{a}_{x_1}^\dagger(y) + \hat{a}_{x_1}(y))}{|x_2-y|^2} + \int_{S_2} dy\, \hat{a}_{x_1}^\dagger(y)\hat{a}_{x_1}(y) \\
& - \frac{\alpha}{\pi^2|x_1 \cdot n|} - \frac{\alpha}{\pi^2|x_2 \cdot n|} - \frac{2\alpha}{|x_1-x_2|}\,, \tag{A.6}
\end{aligned}$$

where $|x_i \cdot n|$ is the distance between x_i and the dividing plane, $i = 1, 2$. (The integrals in the last line of Eq. (A.4) can be done explicitly via cylindrical coordinates, resulting in the first and second terms in the last line of this identity; the last term is an integral of $|x_1 - y|^{-2}|x_2 - y|^{-2}$ over *all* of $\mathbb{R}^3$ and is readily computed to be the Coulomb attraction term.)

We can give a lower bound on expectations of the right side of the first line of this last equation (A.6), assuming the first particle is indeed confined in the ball

B_1. Let K_{S_1,x_2} be the one-particle operator of the first line,

$$K_{S_1,x_2} = p_1^2 - \frac{\sqrt{\alpha}}{\pi^{3/2}} \int_{S_1} dy \, \frac{\hat{a}_{x_2}^{\dagger}(y) + \hat{a}_{x_2}(y)}{|x_1 - y|^2} + \int_{S_1} dy \, \hat{a}_{x_2}^{\dagger}(y) \hat{a}_{x_2}(y) \,, \qquad (A.7)$$

which we regard as acting in the Hilbert space $L^2(S_1) \otimes \mathcal{F}_{S_1}$, the latter factor being the Fock space associated with the phonon variables $y \in S_1$; the operator is a function of $x_2 \in S_2$. Note that p_1 commutes with $\hat{a}_{x_2}(y)$ and its adjoint and that $\hat{a}_{x_2}(y)$ and $\hat{a}_{x_2}^{\dagger}(y)$ satisfy the canonical commutation relations. The operator function K_{S_2,x_1} is defined analogously.

Fix x_2, let ψ be a state in $L^2(\mathbb{R}^3) \otimes \mathcal{F}_{S_1}$ supported in $x_1 \in B_1$, and then consider a product state $\Psi = \psi \otimes \Phi \in L^2(\mathbb{R}^3) \otimes \mathcal{F}$ where Φ is a coherent state of the phonon variables corresponding to $y \in S_2$ such that

$$\hat{a}(y)|\Phi\rangle = \frac{\sqrt{\alpha}}{\pi^{3/2}|x_c - y|^2} \, |\Phi\rangle \,, \ y \in S_2. \qquad (A.8)$$

Here, we take $x_c \in S_1$ to be on the line passing through the centers of the two balls and of distance $d/2 + 2R$ from the dividing plane (i.e. as remote from the dividing plane as possible but on the surface of B_1). For such a state Ψ, we have that

$$E^{(1)}(\alpha) \leq \langle \Psi | H^{(1)} | \Psi \rangle$$

$$= \langle \psi | K_{S_1,x_2} | \psi \rangle - \frac{2\alpha}{\pi^3} \int_{S_2} dy \left\langle \psi \left| \frac{1}{|x_1 - y|^2 |x_c - y|^2} \right| \psi \right\rangle + \frac{\alpha}{\pi^3} \int_{S_2} \frac{dy}{|x_c - y|^4}$$

$$\leq \langle \psi | K_{S_1,x_2} | \psi \rangle - \frac{2\alpha}{\pi^3} \inf_{x_1 \in B_1} \int \frac{dy}{|x_1 - y|^2 |x_c - y|^2} + \frac{\alpha}{\pi^3(d/2 + 2R)} \,. \quad (A.9)$$

The integral in the infimum is seen to have no critical points for x_1 in the interior of B_1 and so attains its minimum for x_1 on the boundary of B_1. The integral can again be written using cylindrical coordinates and the angular integration performed explicitly. One then writes the integrand of the resulting double integral just as a function of z_1, say, where $x_1 = (r_1, \theta_1, z_1)$ in cylindrical coordinates, and where $(z_1 + d/2 + R)^2 + r_1^2 = R^2$. Minimization of the integrand in this double integral regarded as a function of z_1 is tedious but straightforward, the minimum occurring at $x_1 = x_c$. The integral $\int_{S_2} dy \, |x_c - y|^{-4}$ is equal to $\pi/(d/2 + 2R)$ as computed above for Eq. (A.4). Thus, we obtain

$$E^{(1)}(\alpha) \leq \langle \psi_1 | K_{S_1,x_2} | \psi_1 \rangle - \frac{\alpha}{\pi^2(d/2 + 2R)}. \qquad (A.10)$$

Of course the second line of Eq. (A.6) is handled similarly.

By this last inequality (A.10) and Eq. (A.6), we have that for any state Ψ with electron support in $B_1 \times B_2$,

$$\langle \Psi | H^{(2)}_{U=0} | \Psi \rangle = \langle \Psi | K_{S_1,x_2} \otimes 1 | \Psi \rangle + \langle \Psi | K_{S_2,x_1} \otimes 1 | \Psi \rangle$$

$$- \alpha \left\langle \Psi \left| \left(\frac{1}{\pi^2 |x_1 \cdot n|} + \frac{1}{\pi^2 |x_2 \cdot n|} + \frac{2}{|x_1 - x_2|} \right) \right| \Psi \right\rangle$$

$$\geq 2E^{(1)}(\alpha) + \frac{2\alpha}{\pi^2(d/2 + 2R)}$$

$$- \alpha \left\langle \Psi \left| \left(\frac{1}{\pi^2 |x_1 \cdot n|} + \frac{1}{\pi^2 |x_2 \cdot n|} + \frac{2}{|x_1 - x_2|} \right) \right| \Psi \right\rangle. \qquad (A.11)$$

Noting that $|x_1 \cdot n|$ and $|x_2 \cdot n|$ are at least $d/2$, we have that

$$\langle\Psi|H_{U=0}^{(2)}|\Psi\rangle \geq 2E^{(1)}(\alpha) - 2\alpha\Big\langle\Psi\Big|\frac{1}{|x_1-x_2|}\Big|\Psi\Big\rangle - \frac{16\alpha R}{\pi^2 d(d+4R)}\,, \qquad (A.12)$$

which is the claim of Lemma 3. $\hfill\square$

References

[1] A. S. Alexandrov, J. T. Devreese, *Advances in polaron physics*. Springer (2010).

[2] F. Brosens, S. N. Klimin, J. T. Devreese, *Variational path-integral treatment of a translation invariant many-polaron system*. Phys. Rev. B **71** (2005), 214301–214313.

[3] J. G. Conlon, E. H. Lieb, H.-T. Yau, *The $N^{7/5}$ law for charged bosons*. Comm. Math. Phys. **116** (1988), 417–448 .

[4] H. L. Cycon, R. G. Froese, W. Kirsch, B. Simon, *Schrödinger operators*. Springer Texts and Monographs in Physics (1987).

[5] J. Dolbeault, A. Laptev, M. Loss, *Lieb-Thirring inequalities with improved constants*. J. Eur. Math. Soc. (JEMS) **10** (2008), no. 4, 1121–1126.

[6] M. Donsker, S. R. S. Varadhan, *Asymptotics for the polaron*. Comm. Pure Appl. Math. **36** (1983), 505–528.

[7] R. P. Feynman, *Slow electrons in a polar crystal*. Phys. Rev. **97**, 660–665 (1955).

[8] R. L. Frank, E. H. Lieb, R. Seiringer, L. E. Thomas, *Bi-polaron and N-polaron binding energies*. Phys. Rev. Lett., to appear. arXiv:1004.1196

[9] H. Fröhlich, *Theory of electrical breakdown in ionic crystals*. Proc. R. Soc. Lond. A **160** (1937), 230–241.

[10] J. Fröhlich, *Existence of dressed one-electron states in a class of persistent models*. Fortschr. Phys. **22** (1974), 159–198.

[11] B. Gerlach, H. Löwen, *Absence of phonon-induced localization for the free optical polaron and the corresponding Wannier exciton-phonon system*. Phys. Rev. B **37** (1988), 8042–8047.

[12] B. Gerlach, H. Löwen, *Analytical properties of polaron systems or: Do polaronic phase transitions exist or not?* Rev. Mod. Phys. **63** (1991), 63–90.

[13] M. Griesemer, J. S. Møller, *Bounds on the minimal energy of translation invariant N-polaron systems*. Comm. Math. Phys., to appear. Preprint (2009), arXiv:0907.0752v1.

[14] M. Gurari, *Self-energy of slow electrons in polar materials*. Phil. Mag. Ser. 7 **44**:350 (1953), 329–336.

[15] M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, *Schrödinger inequalities and asymptotics behavior of the electron density of atoms and molecules*. Phys. Rev. A **16** (1977), 1782–1785.

[16] T-D. Lee, D. Pines, *The motion of slow electrons in polar crystals*. Phys. Rev. **88** (1952), 960–961.

[17] T-D. Lee, F. Low, D. Pines, *The motion of slow electrons in a polar crystal*. Phys. Rev. **90** (1953), 297–302.

[18] E. H. Lieb, *Existence and uniqueness of the minimizing solution of Choquard's nonlinear equation*. Studies in Appl. Math. **57** (1976/77), no. 2, 93–105.

[19] E. H. Lieb, S. Oxford, *An improved lower bound on the indirect Coulomb energy*. Int. J. Quant. Chem. **19** (1981), 427–439.

[20] E. H. Lieb, R. Seiringer, *The stability of matter in quantum mechanics*. Cambridge (2010).

[21] E. H. Lieb, J.P. Solovej, *Ground state energy of the one-component charged bose gas*. Comm. Math. Phys. **217** (2001), 127–163. Erratum: ibid. **225** (2002), 219–221.

[22] E. H. Lieb, W. Thirring, *Bound for the kinetic energy of fermions which proves the stability of matter*. Phys. Rev. Lett. **35** (1975), 687–689. Erratum: ibid. **35** (1975), 1116.

[23] E. H. Lieb, L. E. Thomas, *Exact ground state energy of the strong-coupling polaron*. Comm. Math. Phys. **183**, no. 3, 511–519 (1997). Erratum: *ibid.* **188**, no. 2, 499–500 (1997).

[24] E. H. Lieb, K. Yamazaki, *Ground-state energy and effective mass of the polaron*. Phys. Rev. **111**, 728–722 (1958).

[25] S. J. Miyake, *Strong coupling limit of the polaron ground state*. J. Phys. Soc. Jpn. **38** (1975), 181–182.

[26] T. Miyao, H. Spohn, *The bipolaron in the strong coupling limit*. Ann. Henri Poincaré **8** (2007), 1333–1370.

[27] J. S. Møller, *The polaron revisited*. Rev. Math. Phys. **18** (2006), no. 5, 485–517.

[28] S. I. Pekar, *Research in electron theory of crystals*. United States Atomic Energy Commission, Washington, DC, 1963.

[29] S. I. Pekar, O. F. Tomasevich, *Theory of F centers*. Zh. Eksp. Teor. Fys. **21** (1951), 1218–1222.

[30] G. Roepstorff, *Path integral approach to quantum physics*. Berlin-Heidelberg-New York, Springer, 1994.

[31] M. A. Smondyrev, V.M. Fomin, *Pekar-Fröhlich bipolarons*. In: *Polarons and applications*, Proceedings in Nonlinear Science, V.D. Lakhno, ed., Wiley (1994).

[32] H. Spohn, *The polaron functional integral*. In: Stochastic processes and their applications, Dordrecht-Boston-London, Kluwer, 1990.

[33] G. Verbist, M. A. Smondyrev, F. M. Peeters, J. T. Devreese, *Strong-coupling analysis of large bipolarons in two and three dimensions*. Phys. Rev. B **45**, 5262–5269 (1992).

R.L. Frank, Department of Mathematics, Princeton University, Washington Road, Princeton, NJ 08544, USA
   E-mail address: `rlfrank@math.princeton.edu`

E.H. Lieb, Departments of Mathematics and Physics, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA
   E-mail address: `lieb@princeton.edu`

R. Seiringer, Department of Physics, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA
   E-mail address: `rseiring@princeton.edu`

L.E. Thomas, Department of Mathematics, University of Virginia, Charlottesville, VA 22904, USA
   E-mail address: `let@virginia.edu`